LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112918\
Data File : VN052560.D
Acq On : 29 Nov 2018 13:05
Operator : MD\SY
Sample : J6065-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : USTS-1-2-3

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.555	842	865	895	rBV2	368633	1120654	17.77%	2.180%
2	7.593	1790	1810	1821	rBV	804519	2013337	31.92%	3.917%
3	7.667	1821	1833	1853	rVB	1535408	3632383	57.59%	7.067%
4	8.027	1927	1945	1975	rBV	819155	1920746	30.45%	3.737%
5	8.165	1976	1988	1997	rBV2	32023	68275	1.08%	0.133%
6	8.587	2101	2119	2149	rBV	2196599	4538165	71.96%	8.830%
7	9.188	2293	2306	2317	rBV2	40902	88856	1.41%	0.173%
8	9.268	2317	2331	2359	rBV	2406725	4483783	71.09%	8.724%
9	9.905	2514	2529	2546	rBV	632599	1089105	17.27%	2.119%
10	10.091	2573	2587	2601	rBV	3517927	6306917	100.00%	12.271%
11	10.281	2636	2646	2667	rVB2	64773	116913	1.85%	0.227%
12	10.545	2712	2728	2744	rBV	417737	712110	11.29%	1.386%
13	10.638	2747	2757	2773	rVV3	155612	272466	4.32%	0.530%
14	10.722	2773	2783	2786	rVV	46338	67867	1.08%	0.132%
15	10.767	2786	2797	2815	rVV	2107722	3466348	54.96%	6.744%
16	10.854	2815	2824	2844	rVB	150888	266083	4.22%	0.518%
17	11.169	2907	2922	2946	rBV	2189332	3465361	54.95%	6.742%
18	11.410	2979	2997	3021	rVB	2933892	5182277	82.17%	10.083%
19	11.619	3051	3062	3074	rBV	35723	68354	1.08%	0.133%
20	11.879	3130	3143	3155	rBV	105914	173636	2.75%	0.338%
21	12.403	3291	3306	3324	rBV	2282883	3834698	60.80%	7.461%
22	13.345	3585	3599	3617	rBV	2503114	4092999	64.90%	7.963%
23	13.545	3654	3661	3671	rVB	52518	81660	1.29%	0.159%
24	13.889	3758	3768	3778	rBV	142653	224527	3.56%	0.437%
25	13.998	3792	3802	3818	rVB2	301409	498336	7.90%	0.970%
26	14.214	3853	3869	3888	rBV	183175	322254	5.11%	0.627%
27	14.480	3944	3952	3961	rBV4	67100	115446	1.83%	0.225%
28	14.596	3975	3988	3999	rBV2	557270	947513	15.02%	1.844%
29	14.660	3999	4008	4017	rVB5	36991	69268	1.10%	0.135%
30	14.850	4051	4067	4074	rBV4	196413	415072	6.58%	0.808%
31	14.886	4075	4078	4087	rVV2	115643	167413	2.65%	0.326%
32	14.959	4089	4101	4119	rVB3	246239	552317	8.76%	1.075%
33	15.136	4148	4156	4168	rVB	66414	114701	1.82%	0.223%
34	15.242	4181	4189	4196	rBV5	33358	64625	1.02%	0.126%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112918\
Data File : VN052560.D
Acq On : 29 Nov 2018 13:05
Operator : MD\SY
Sample : J6065-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : USTS-1-2-3

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Title : SW846 8260

35	15.294	4197	4205	4222	rVB2	75440	152905	2.42%	0.297%
36	15.419	4233	4244	4257	rBV	133789	240228	3.81%	0.467%
37	15.580	4280	4294	4314	rBV3	98060	251872	3.99%	0.490%
38	15.702	4322	4332	4342	rBV2	44352	83161	1.32%	0.162%
39	15.773	4342	4354	4364	rVB4	53320	114670	1.82%	0.223%

Sum of corrected areas: 51397301

LSC Report - Integrated Chromatogram

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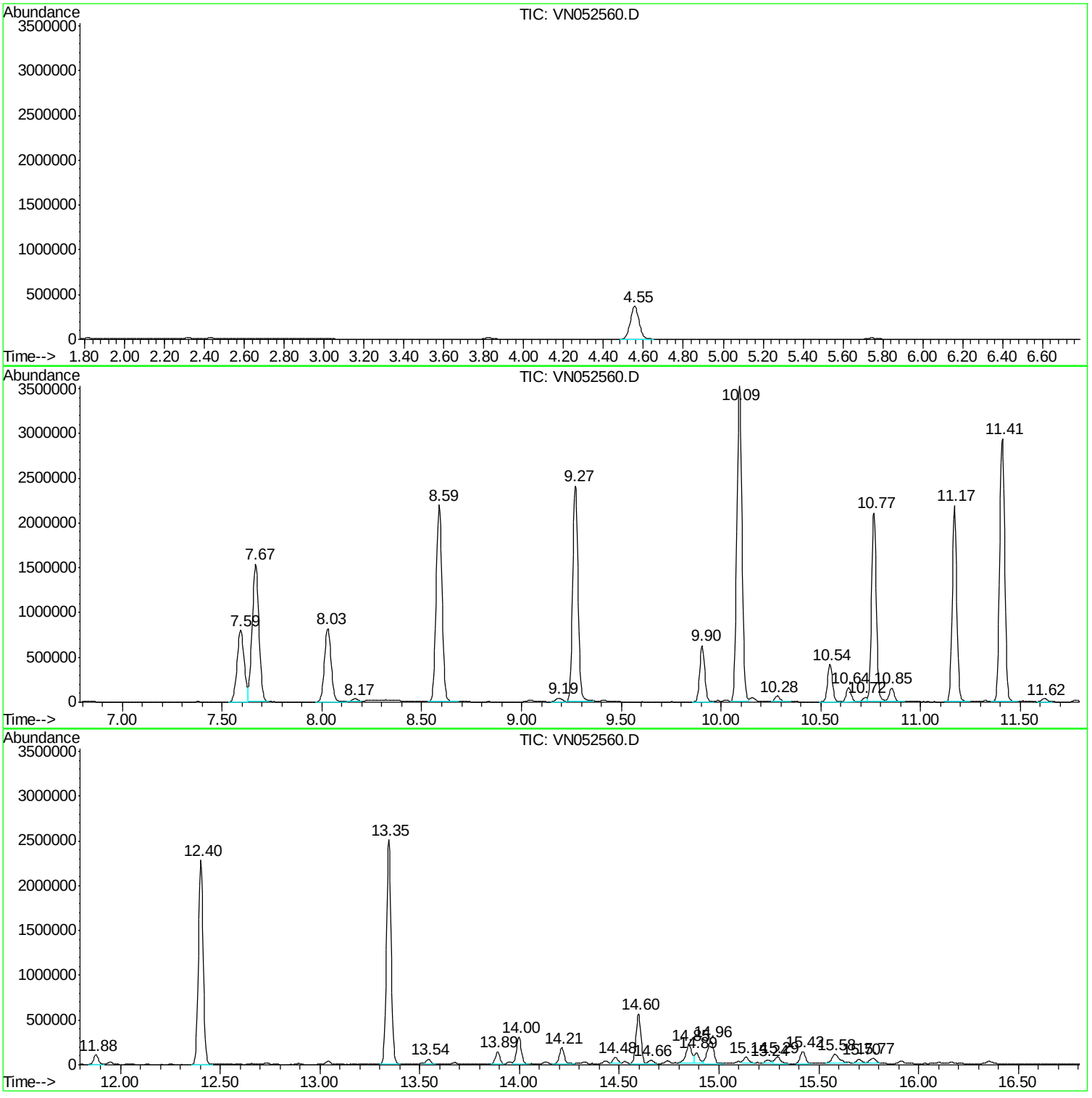
Data File : VN052560.D
Acq On : 29 Nov 2018 13:05
Operator : MD\SY
Sample : J6065-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
USTS-1-2-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112918\
Data File : VN052560.D
Acq On : 29 Nov 2018 13:05
Operator : MD\SY
Sample : J6065-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : USTS-1-2-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

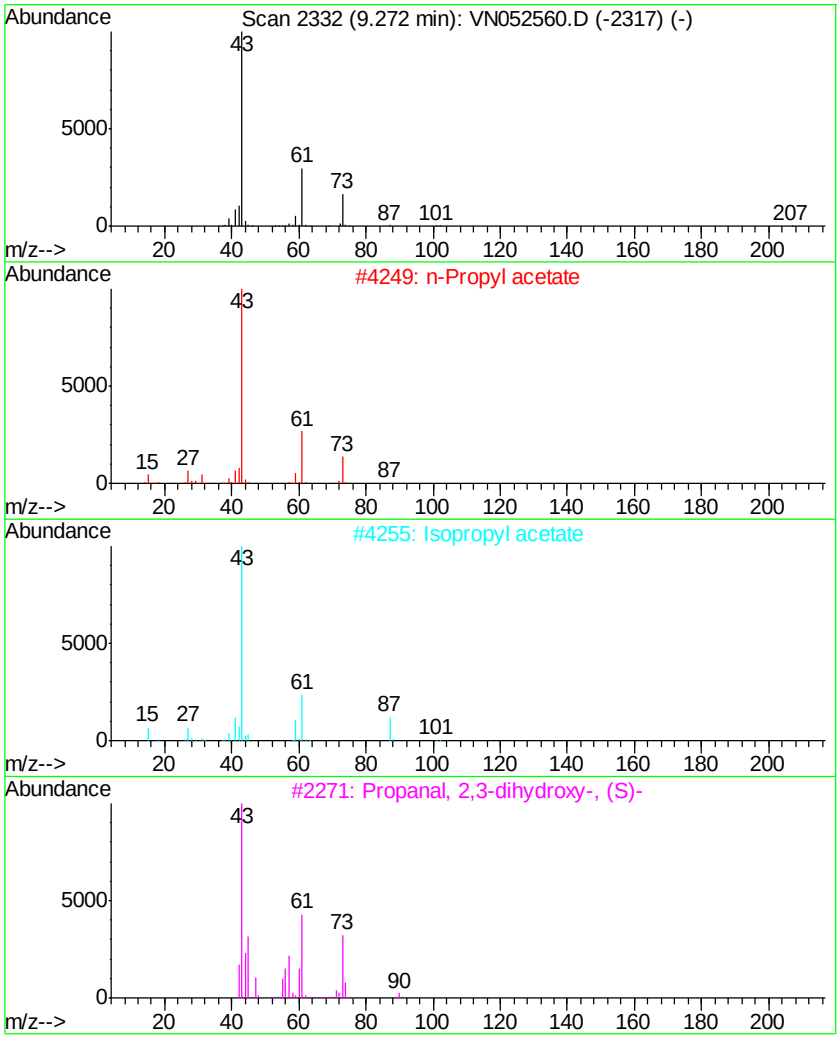
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

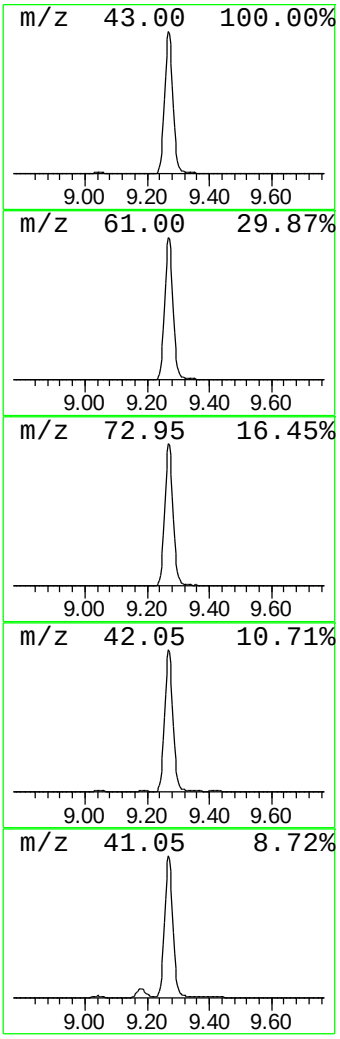
****

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.27	49.40 ug/l	4483780	1,4-Difluorobenzene	8.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	Isopropyl acetate	102	C5H10O2	000108-21-4	36
3	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	9
4	1-Butanamine	73	C4H11N	000109-73-9	7
5	Isobutylamine	73	C4H11N	000078-81-9	5





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112918\
Data File : VN052560.D
Acq On : 29 Nov 2018 13:05
Operator : MD\SY
Sample : J6065-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : USTS-1-2-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

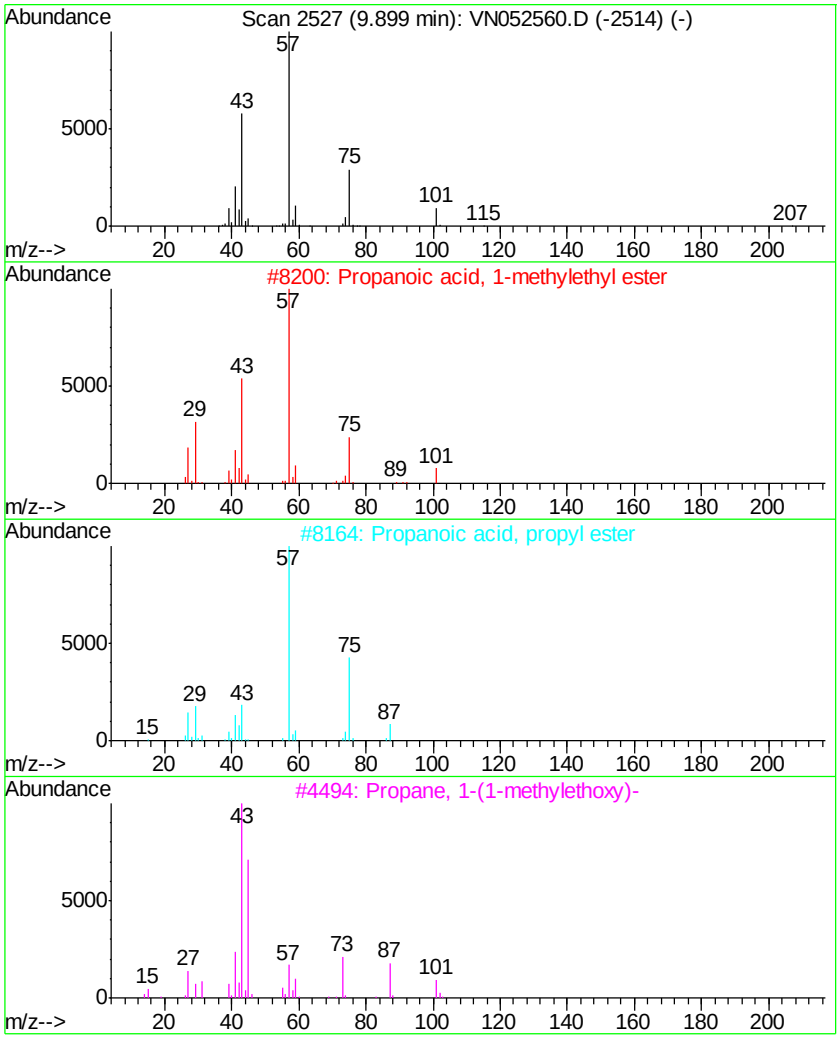
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

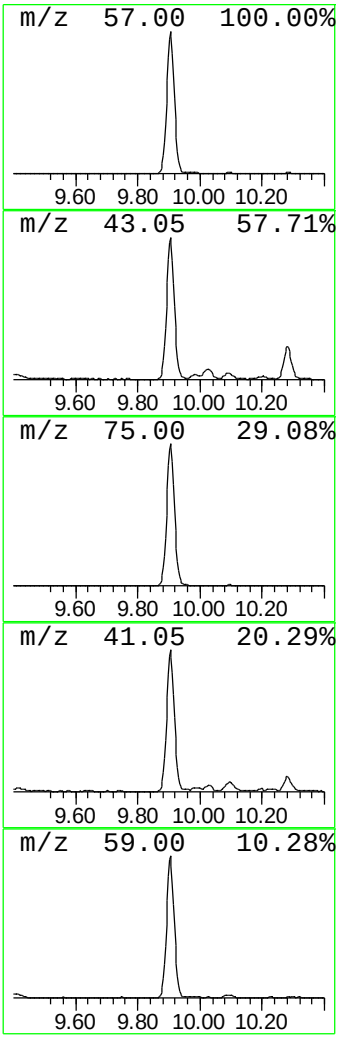
****

Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.90	12.00 ug/l	1089110	1,4-Difluorobenzene	8.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	36
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112918\
Data File : VN052560.D
Acq On : 29 Nov 2018 13:05
Operator : MD\SY
Sample : J6065-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : USTS-1-2-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

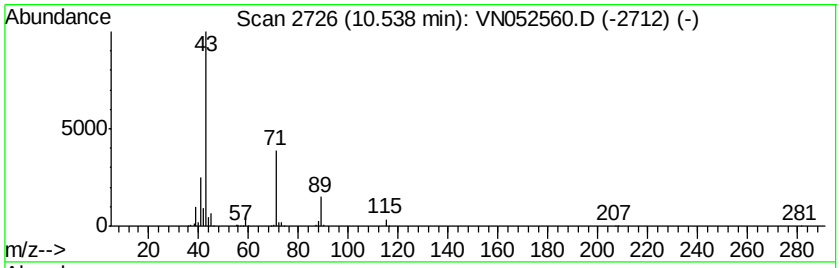
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

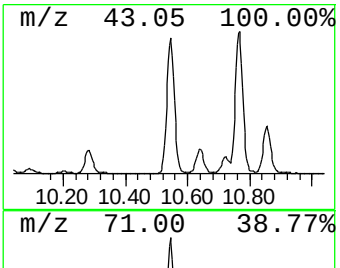
****

Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.54	6.87 ug/l	712110	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	72
4	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	38
5	1,4-Butanediamine	88	C4H12N2	000110-60-1	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112918\
Data File : VN052560.D
Acq On : 29 Nov 2018 13:05
Operator : MD\SY
Sample : J6065-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : USTS-1-2-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

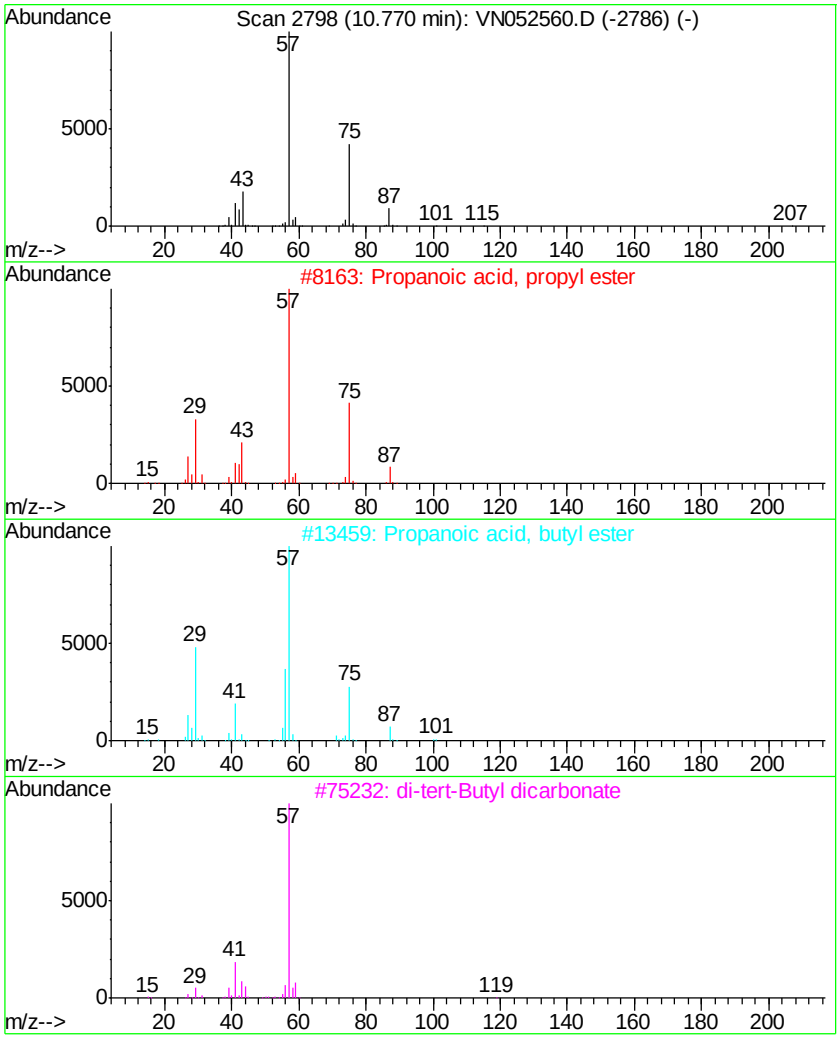
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

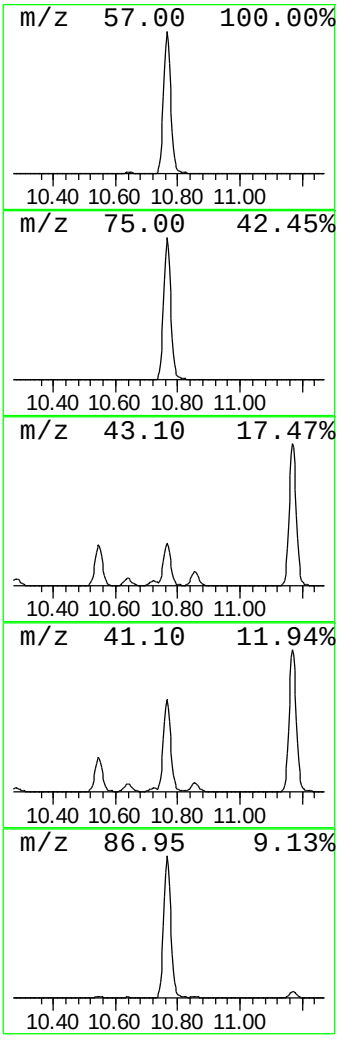
****

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	33.44 ug/l	3466350	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
3	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
4	1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	7
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112918\
Data File : VN052560.D
Acq On : 29 Nov 2018 13:05
Operator : MD\SY
Sample : J6065-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : USTS-1-2-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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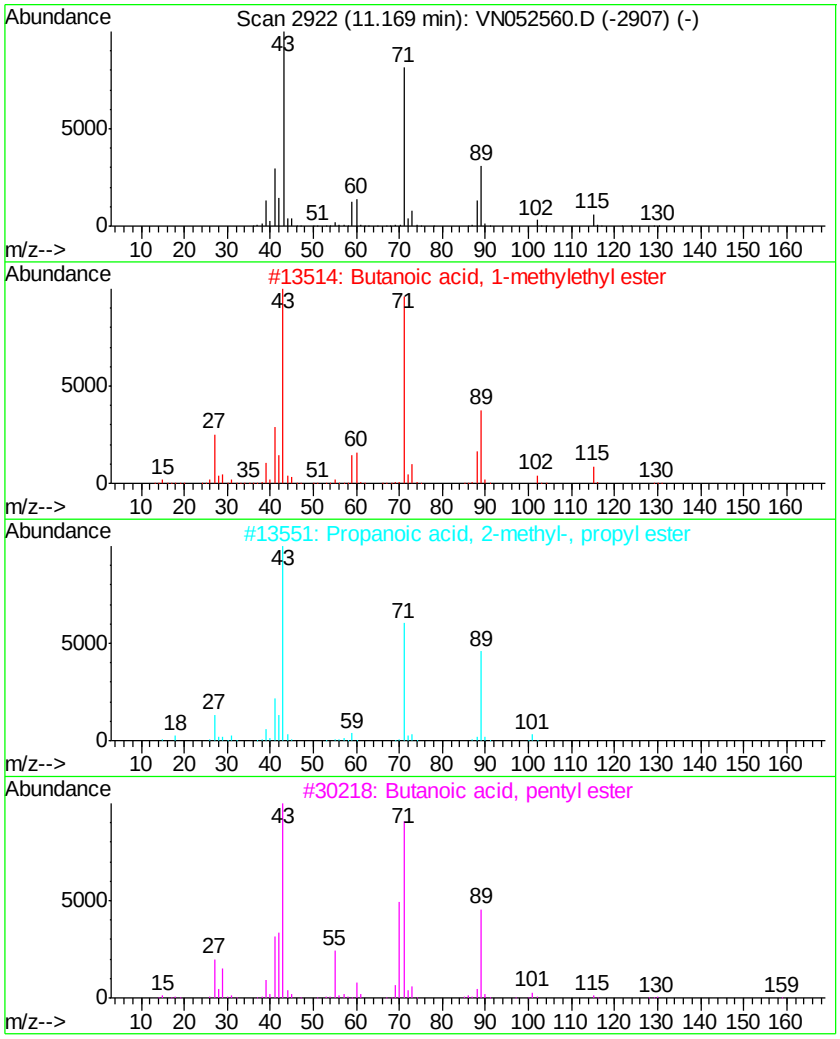
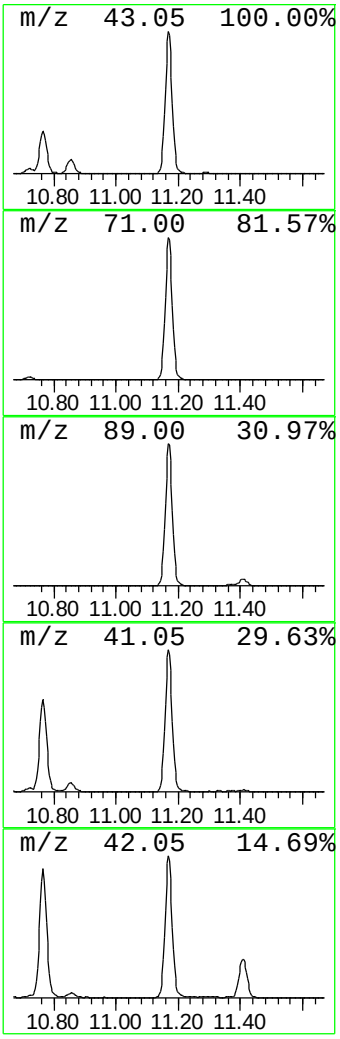
****

Peak Number 5 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.17	33.43 ug/l	3465360	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112918\
Data File : VN052560.D
Acq On : 29 Nov 2018 13:05
Operator : MD\SY
Sample : J6065-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : USTS-1-2-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

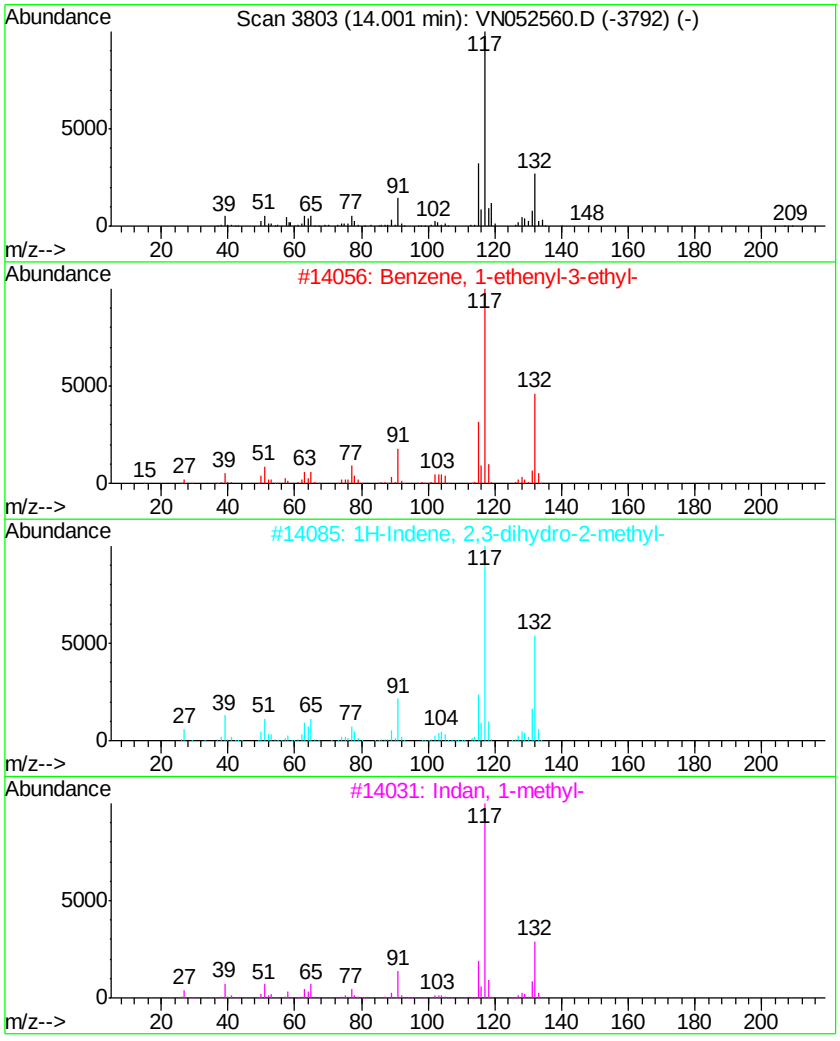
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

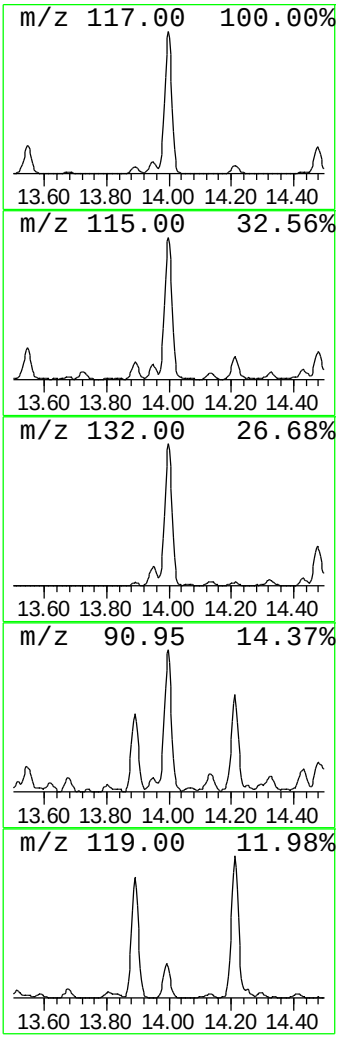
****

Peak Number 6 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	6.09 ug/l	498336	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
2	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	83
3	Indan, 1-methyl-	132	C10H12	000767-58-8	81
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	80
5	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	80





Library Search Compound Report

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Sample : J6065-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : USTS-1-2-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

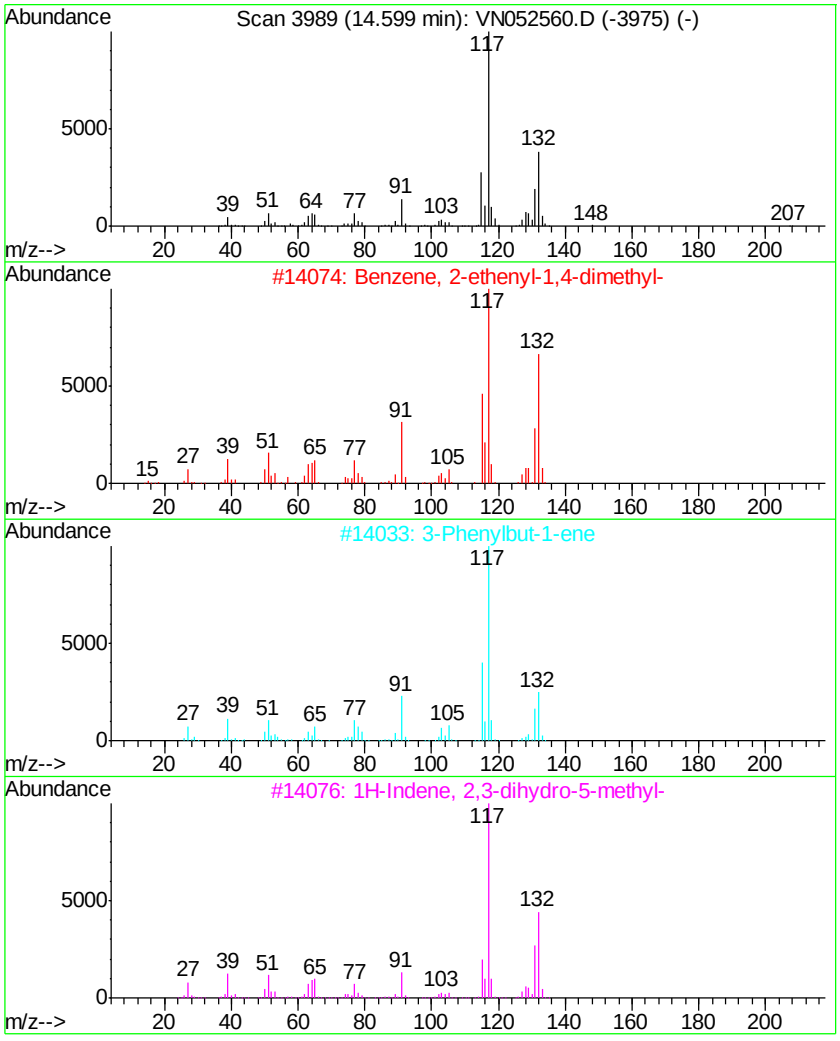
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

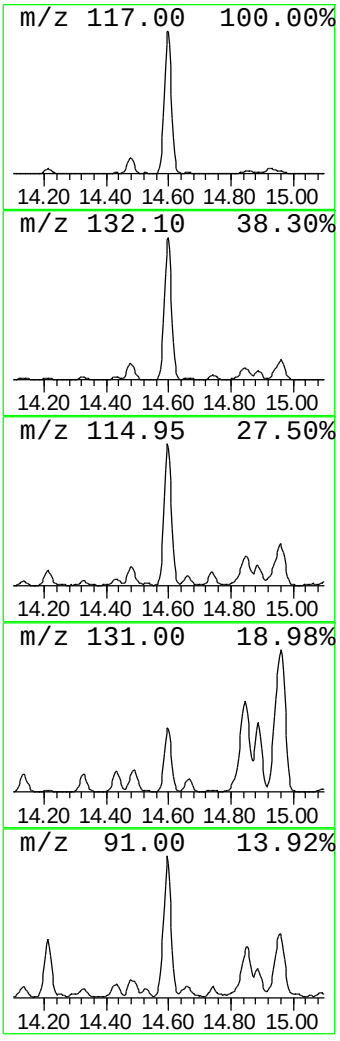
****

Peak Number 7 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	11.57 ug/l	947513	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
4	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	90
5	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90





Library Search Compound Report

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Data File : VN052560.D
Acq On : 29 Nov 2018 13:05
Operator : MD\SY
Sample : J6065-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : USTS-1-2-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

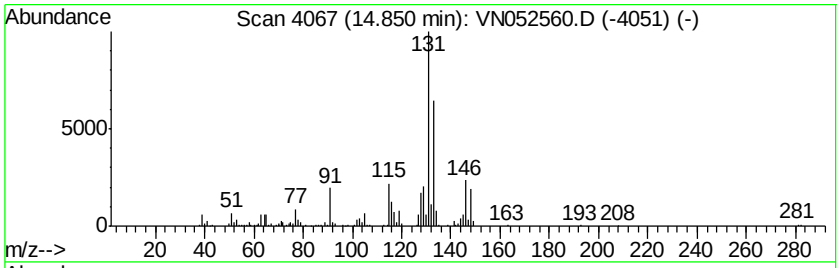
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

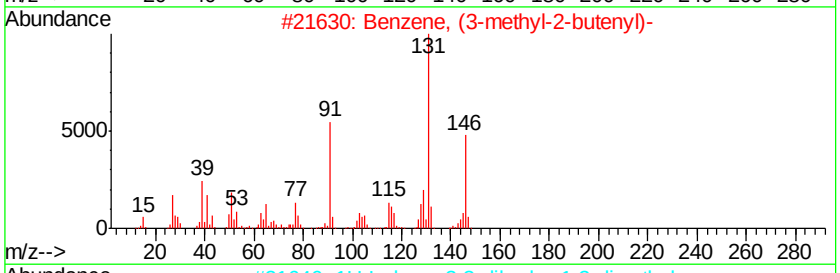
****

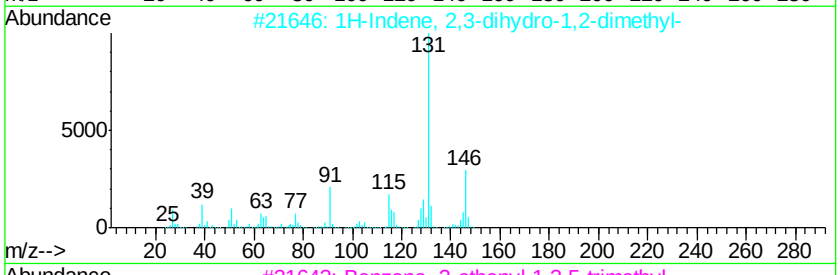
Peak Number 8 Benzene, (3-methyl-2-butenyl)- Concentration Rank 9

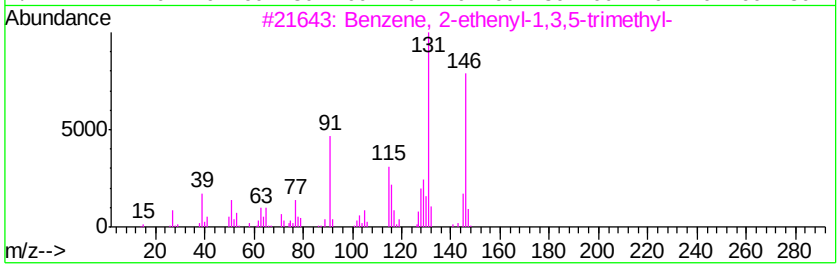
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	5.07 ug/l	415072	1,4-Dichlorobenzene-d4	13.35

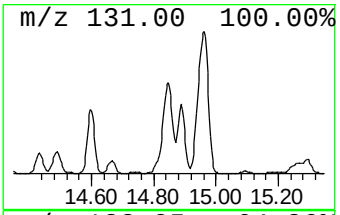
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	93
2	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	93
3	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	76
4	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	70
5	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	70

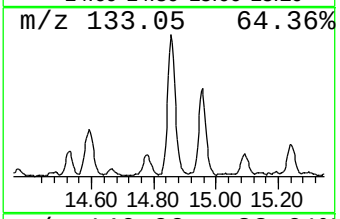


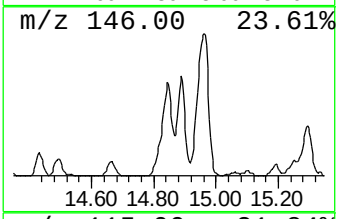


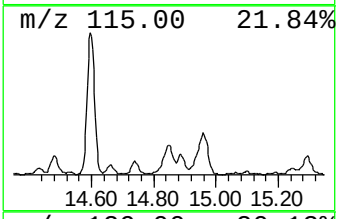


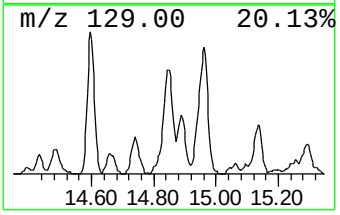












Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112918\
Data File : VN052560.D
Acq On : 29 Nov 2018 13:05
Operator : MD\SY
Sample : J6065-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : USTS-1-2-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

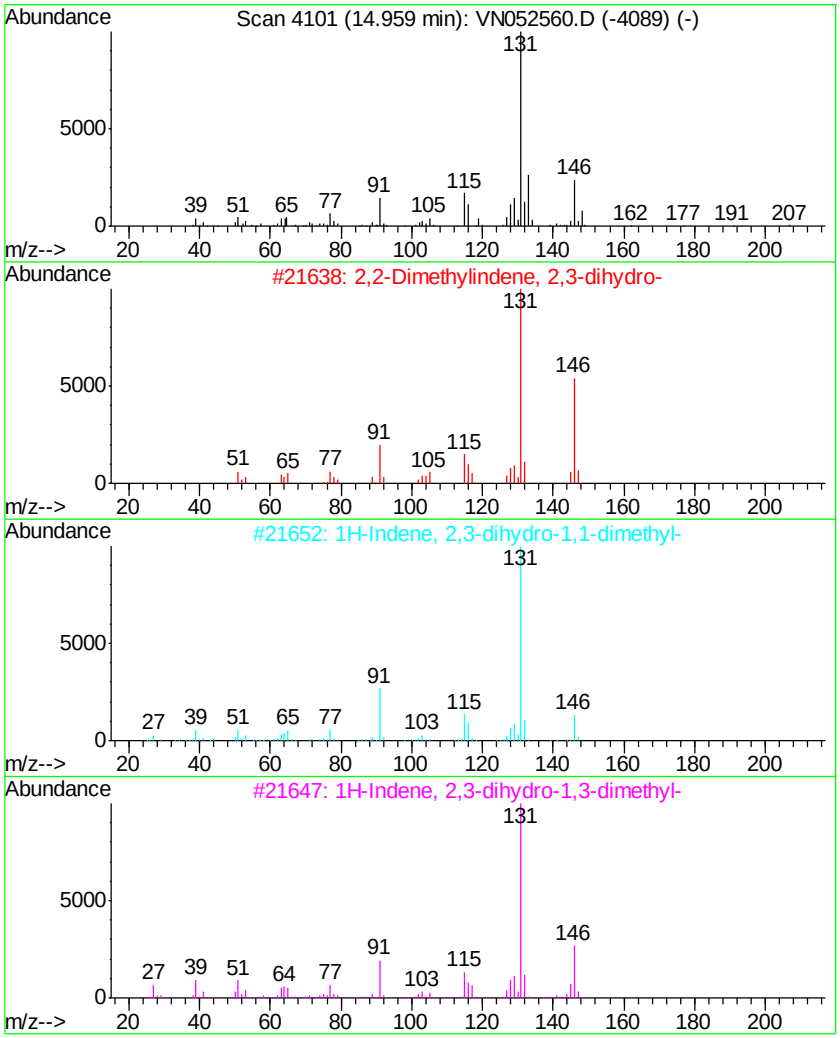
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

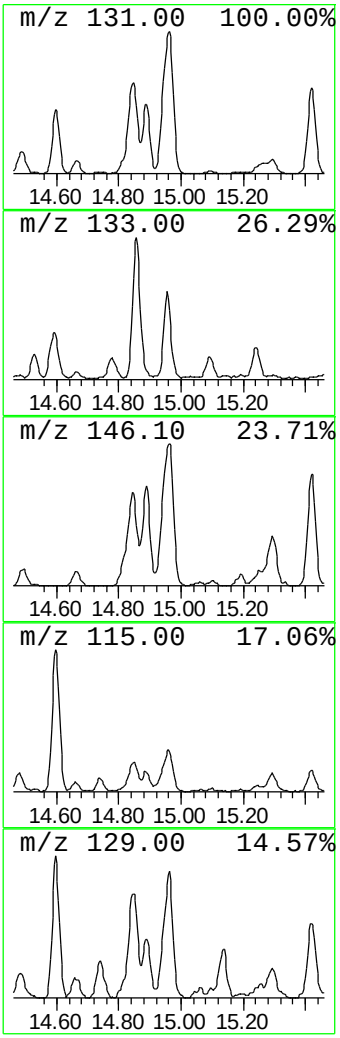
****

Peak Number 9 2,2-Dimethylindene, 2,3-dih... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	6.75 ug/l	552317	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	87
2	1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	87
3	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	87
4	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	87
5	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112918\
Data File : VN052560.D
Acq On : 29 Nov 2018 13:05
Operator : MD\SY
Sample : J6065-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : USTS-1-2-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	9.27	49.4	ug/l	4483780	2	8.59	4538170	50.0
Propanoic acid, 1...	9.90	12.0	ug/l	1089110	2	8.59	4538170	50.0
Propanoic acid, 2...	10.54	6.9	ug/l	712110	3	11.41	5182280	50.0
Propanoic acid, p...	10.77	33.4	ug/l	3466350	3	11.41	5182280	50.0
Butanoic acid, 1-...	11.17	33.4	ug/l	3465360	3	11.41	5182280	50.0
Benzene, 1-etheny...	14.00	6.1	ug/l	498336	4	13.35	4093000	50.0
Benzene, 2-etheny...	14.60	11.6	ug/l	947513	4	13.35	4093000	50.0
Benzene, (3-methy...	14.85	5.1	ug/l	415072	4	13.35	4093000	50.0
2,2-Dimethylinden...	14.96	6.8	ug/l	552317	4	13.35	4093000	50.0